Propagation of neutron de Broglie waves inside the slot cut in a single Si crystal

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ABSTRACT

It was recently proposed by Dombeck et al to search for a Neutron Electric Dipole Moment (EDM) by means of the neutron multiple Bragg back-scattering. The dynamical diffraction analysis of the proposed experiment is the subject of this paper. The neutron wave modes were calculated for the case of the infinitely long slot cut inside of a thick Si crystal parallel to the crystallographic planes and placed in a steady magnetic field. The calculated neutron modes have a discrete spectrum of a momenta along the direction of the slot axis. The external magnetic field causes some particular discrete modes to become degenerate. However, the Schwinger and EDM interactions of neutrons with the slot walls break this degeneracy, which in turn leads to the complicated motion of the neutron polarization vector along the slot axis. The spin deviation from the starting direction is accumulated during neutron motion in slot. The energy spectrum of neutrons transmitted through the slot contains several peaks instead of one existing for the case of the ultra back-scattering regime.

Keywords: neutron, resonator, slot, crystal, back-scattering, EDM, Schwinger interaction.

1. INTRODUCTION

During recent years then has been increased interest in the research on devices which utilize multiply Bragg diffraction from perfect single crystals. Successful experiments concerning neutron storage, that is confinement of the thermal neutrons between two back reflected, $\theta_B=\pi/2$ perfect silicon single crystals is an example [1]. The problem here is one in which the neutron is moving horizontally between these back reflecting vertical silicon mirrors and is confined by means of the neutron guide walls. Finkelstein [2,3] observed the Spin-orbit (Schwinger) interaction between the neutron spin and crystalline electric field in a silicon single crystal placed in the external magnetic field. This magnetic field led to the degeneracy of the neutron states belonging to the different spin orientations and simultaneously to the different branches of the neutron dispersion surface in silicon. These degenerate states are very sensitive with respect to small perturbations. This circumstance allowed the observation of the Schwinger interaction, which is usually 4 orders smaller than the nuclear interaction between the neutron and silicon lattice [2]. The condition for the above mentioned degeneracy is written in the very simple form for the case of Laue diffraction,

$$\frac{\omega_Z \tau}{v \cos \theta_B} = 2\pi \tag{1}$$

where ω_Z, v is neutron Zeeman frequency and velocity, respectively. θ_B is the Bragg angle and τ is an extinction length. The relatively strong homogeneous magnetic field was used in this experiment, H=6279.3 Gauss [2].

Recently Dombeck et al [4] proposed to use the multiply Bragg Back Scattering (BS) from the slot cut in the single crystal for the Neutron Electric Dipole Moment (EDM) search. The neutron spin is disturbed by EDM or Schwinger interactions in the slot wall and rotates at the angle π during the transit from one slot side to the another, so that the effect of perturbation is accumulating during multiply, $\sim10^4$ reflections from the slot walls. Dombeck et al [4] used the simple geometrical optics approach in order to make necessary estimates.

The dynamical diffraction analysis of the proposed experiment [4] is the subject of this paper. The neutron wave modes are calculated for the case of the infinitely long slot cut inside of a thick Si crystal parallel to the (111) or (220) crystallographic planes. We call such a crystal placed in the steady homogeneous magnetic field a Wave Guidance-Resonator (WGR). The calculated neutron modes have a discrete spectrum of the momenta, Q, in the direction of the slot axis. The external magnetic field causes some particular discrete modes to become degenerate. However, the Schwinger and EDM interactions

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of neutrons with the WGR walls break this degeneracy, which in turn leads to the complicated motion of the neutron polarization vector along the WGR axis. Calculations were carried out for the two cases: a) the conventional BS; b) Ultra-Back Scattering (UBS), $2\theta_B \approx \pi$. The energy resolution, ΔE, of conventional BS spectrometers is limited by the value of $\Delta E \sim \Delta k_0 v$, even in the UBS regime (Δk_0 is the gap between the branches of the neutron dispersion surface and v is the neutron velocity). However the value of Q is discrete for the WGR regime, which leads to the appearance of several narrow peaks in the energy spectrum of neutrons transmitted along the slot.

The general formulation of model (the neutron WGR placed in the magnetic field) is done in the part 2 of this paper. We calculate discrete neutron modes and the condition of their degeneracy. The cumbersome calculations of the effects of small EDM are presented in the part 3. The Schwinger interaction effect is described in part 4. In part 5 we show how our results can be reformulated for the case of Ultra Back Scattering regime, $2\theta_B \approx \pi$. The brief discussion of the results is done in the Conclusion.

2. NEUTRON WAVE GUIDANCE RESONATOR MODEL

We consider the neutron de Broglie wave propagation in a slot cut in a Si single crystal and along X-axis (see Figure 1). The Y-axis is perpendicular to the slot surface and collinear to the scattering vector **G**. The Z-axis is perpendicular to the plane of scattering. The neutron WGR is placed in a external homogenous magnetic field **H**. Here we first do not take into account weak EDM and Schwinger interactions This will be done in part 3. Therefore, the doubled spin projection, α at the direction of **H** is conserved and we can limit ourselves by the ordinary two waves approximation of the dynamic scattering theory [4,5] The neutron wave function is a superposition of the incident (0) and diffracted (h) parts,

$$\Psi(\alpha) = \Psi_0(\alpha) exp(i\mathbf{k}_0\mathbf{r}) + \Psi_h(\alpha) exp(i\mathbf{k}_h\mathbf{r}); \ \alpha = \pm 1,$$

where

$$\mathbf{k}_0 = k_0(cos\ \theta_B, sin\ \theta_B, 0), \quad \mathbf{k}_h = k_0(cos\ \theta_B, -sin\ \theta_B, 0)$$

and (2)

$$\mathbf{k}_h = \mathbf{k}_0 + \mathbf{G}, G = 2k_0\ sin\ \theta_B$$

$\Psi_0(\alpha)$, $\Psi_h(\alpha)$ can be find by means of dynamical diffraction theory equations:

$$-i\hbar^2/m(\mathbf{k}_0\nabla)\Psi_0(\alpha) + (V_0 - \alpha\hbar\omega_Z/2)\Psi_0(\alpha) + V_{-G}\Psi_h(\alpha) = 0,$$
$$-i\hbar^2/m(\mathbf{k}_h\nabla)\Psi_h(\alpha) + (V_0 - \alpha\hbar\omega_Z/2)\Psi_h(\alpha) + V_G\Psi_0(\alpha) = 0, \quad (3)$$

here m is the neutron mass, ω_Z is neutron Zeeman frequency in the external magnetic field H, V_0, V_G and V_{-G} are Fourier components of the interaction between neutron and Si crystal lattice. The gap Δk_0 between the branches of the neutron dispersion surfaces in the bulk silicon and the extinction length τ can be written in the standard form

$$\Delta k_0 = 2m|V_G|/(\hbar^2 k_0 cos\theta_B), \ \ \tau = 2\pi/\Delta k_0 \quad (4)$$

The equations (3) can be transformed to the convenient dimensionless form after the substitutions

$$x \to x2/\Delta k_0, y \to y2tg(\theta_B)/\Delta k_0, V_G/|V_G| = exp(i\rho_B), \delta = \frac{\omega_Z m\tau}{\hbar\pi k_0 cos\theta_B}, \quad (5a)$$

so that

$$\Psi_0 \to \Psi_0 exp(-i\frac{V_0}{|V_G|}x)exp(-i\rho_B/2), \Psi_h \to \Psi_h exp(-i\frac{V_0}{|V_G|}x)exp(+i\rho_B/2), \quad (5b)$$

and one then has

$$-i(\partial/\partial y + \partial/\partial x)\Psi_0(\alpha) + \Psi_h - \alpha\delta\Psi_0(\alpha) = 0,$$
$$-i(-\partial/\partial y + \partial/\partial x)\Psi_h(\alpha) + \Psi_0 - \alpha\delta\Psi_h(\alpha) = 0 \quad (6)$$

The solution of (6) can be written in the form

$$\Psi_{0,h}=\Phi_{0,h}(\alpha,r)exp(iQx+iP(\alpha,r)y),\ \ r=\pm1,$$

$$Q=\alpha\delta+cos\,\xi,\ \ P(\alpha,r)=ir\sin\xi,\ \ 0<\xi<\pi \tag{7}$$

$$\Phi_0(\alpha,r)exp(ir\xi)+\Phi_h(\alpha,r)=0, \tag{8}$$

where Q, P are the components of the neutron quasi momentum parallel and perpendicular to the slot surface, respectively. We are interested in the case of the multiple Bragg scattering, so that the neutron cannot penetrate deeply inside the bulk silicon crystal. Therefore we limit ourselves by the solution of (6) corresponding to the case of the neutron total reflection from the slot walls, that is $0<\xi<\pi$. The relation (8) can be considered as boundary condition at the slot wall at $y=rD/2$, where D is slot width.

Scattering is absent inside the slot and the corresponding wave function, taking into account (5b), can be found from the equations

$$-i(\partial/\partial y+\partial/\partial x)\Psi_0(\alpha)+(-V_0/|V_G|-\alpha\delta)\Psi_0(\alpha)=0,$$

$$-i(-\partial/\partial y+\partial/\partial x)\Psi_h(\alpha)+(-V_0/|V_G|-\alpha\delta)\Psi_h(\alpha)=0 \tag{9}$$

which have very simple solutions

$$\Psi_0(\alpha)=F_0\,exp(iQz+iP(\alpha,0)x),\ \ \Psi_h(\alpha)=0,\ \ P(\alpha,0)=-(Q-\alpha\delta-V_0/|V_G|)\ \text{ or}$$

$$\Psi_h(\alpha)=F_h\,exp(iQz+iP(\alpha,h)x),\ \ \Psi_0(\alpha)=0,\ \ P(\alpha,h)=+(Q-\alpha\delta-V_0/|V_G|),$$

$$P(\alpha,0)+P(\alpha,h)=0 \tag{10}$$

F_0, F_h are the components of the wave function at the slot center, y=0. The value of quasi momentum, Q directed along slot axis, is the same inside the slot and the slot walls. The neutron wave function should be continuous at the slot sides. These boundary conditions lead to the relations

$$F_0\,exp(ir\xi)exp(iP(\alpha,0)rD/2)+F_h\,exp(iP(\alpha,h)rD/2)=0,\ \ r=\pm1, \tag{11}$$

Equation (11) have a solution if

$$\xi=\xi_L,\ \ \xi_L-D(cos\,\xi_L-V_0/|V_G|)=\pi L\ ,\ \ L=1,2,...,\ \ Q=\alpha\delta+cos\,\xi_L \tag{12}$$

The expressions (12) demonstrate that the neutron de Broglie wave has a discrete quasi momentum spectrum Q directed along slot axis. The quasi momentum spectrum is continuous for the case of ordinary Bragg reflection from the one perfect crystal surface. The wave function corresponding to the discrete modes is especially simple inside the slot,

$$|\Psi\rangle=\left|\begin{matrix}\Psi_0\\ \Psi_h\end{matrix}\right\rangle=\frac{1}{\sqrt{2}}\left|\begin{matrix}exp(i(\pi L-\xi_L)y/D)\\ exp(i\pi(L+1)-i(L-\xi_L)y/D)\end{matrix}\right\rangle exp\{i(Q-V_0/|V_G|)x\} \tag{13}$$

Two modes with opposite spin orientation will be described by the same values of Q, if two solutions of (12) are given by the relation

$$cos\,\xi_\alpha-cos\,\xi_{-\alpha}=-2\alpha\delta \tag{14}$$

This degeneracy can be achieved by means of changing the value of the external magnetic field and leads to higher sensitivity to the EDM and Schwinger interactions in the slot walls. The parameter $V_0/|V_G|$ is equals to 1 and $2^{1/2}$ for the case of Si(220) and Si(111) reflection, respectively. The dimensionless slot thickness, as a rule, is large, D>>1. The number of the discrete neutron modes, M

$$M\approx2D/\pi \tag{15}$$

For an example, for the case of Si(440) reflection and λ=0.1917 nm, the value of θ_B, $\tau*\tan\theta_B/\pi$ are equal to 87.13° and 25.6 μm, respectively. Therefore for the case of slot width equal to 1 mm the number of neutron modes M=24.

3. EDM EFFECTS

3.1. Neutron reflection from one side of the slot.

A neutron passing near an atomic nucleus will experience a change in kinetic energy, $-\Delta V$, due to the EDM interaction with an electric field existing inside of crystal.

$$\Delta V = -\mu_{EDM}\mathbf{S}\bullet\mathbf{E} \tag{16}$$

where μ_{EDM}, **S** is the neutron EDM and spin, respectively, and **E** is an electric field existing inside of crystal, $E\sim7.6\times10^8$ V/cm. Only one Fourier component $\Delta V(G)$, corresponding to the scattering vector **G**, is important in our case. The corresponding electric field is collinear to the vector **G**, $\Delta V(G)$ can be written in the form

$$\Delta V(G) = -i\mu_{EDM}\mathbf{S}\bullet\mathbf{G}Ze(1-f(G))/(2\pi^2\varepsilon_0 G^2) \tag{17}$$

where Ze is the nuclear charge reduced by the electron screening factor $(1-f(G))$, $f(G)$ is X-ray form-factor, and ε_0 is the dielectric constant [4,7]. It is necessary to emphasize that value of $\Delta V(G)$ is imaginary and is odd for the respect of vector **G**. The value of EDM is very small, $\mu_{EDM}<1.2\times10^{-25}$ e-cm [4]. Therefore is it important that the result of discussed experiment will not be "contaminated" by the more stronger effect induced by the Schwinger interaction between the neutron spin and the electric field, which is proportional to the value of [S·E]. We suppose that the external magnetic field is directed along Z- axis (Figure 1). The effect of Schwinger interaction will be suppressed in this case. The dynamical theory equations are written in the form

$$\begin{aligned} &-i(\partial/\partial y+\partial/\partial x)\Psi_0+\Psi_h-\delta\sigma_Z\Psi_0+iA\sigma_Y\Psi_h=0,\\ &-i(-\partial/\partial y+\partial/\partial x)\Psi_h+\Psi_0-\delta\sigma_Z\Psi_h-iA\sigma_Y\Psi_0=0 \end{aligned} \tag{18}$$

$$A=-\mu_{EDM}S\bullet GZe(1-f)/(4\pi^2\varepsilon_0 G^2),$$

where Ψ_0, Ψ_h are two-components spinors.

$$\begin{aligned} &-i(\partial/\partial y+\partial/\partial x)\Psi_0+\Psi_h-\delta\sigma_Z\Psi_0+iA\sigma_Y\Psi_h=0,\\ &-i(-\partial/\partial y+\partial/\partial x)\Psi_h+\Psi_0-\delta\sigma_Z\Psi_h-iA\sigma_Y\Psi_0=0, \end{aligned} \tag{19}$$

$$\sigma_X=\begin{pmatrix}0,1\\1,0\end{pmatrix},\ \sigma_Y=\begin{pmatrix}0,-i\\i,0\end{pmatrix},\ \sigma_Z=\begin{pmatrix}1,0\\0,-1\end{pmatrix},\ |A|<<1$$

We have equations for the calculation of components $\Psi_{0,h}(\alpha)\exp(iQx+iPy)$, corresponding to the projection α of the neutron spin along the magnetic field direction:

$$\begin{aligned} &(P+Q-\alpha\delta)\Psi_0(\alpha)+\Psi_h(\alpha)+\alpha A\ \Psi_h(-\alpha)=0,\\ &(-P+Q-\alpha\delta)\Psi_h(\alpha)+\Psi_0(\alpha)-\alpha A\Psi_0(-\alpha)=0,\ \alpha=\pm1 \end{aligned} \tag{20}$$

The EDM interaction creates only the very small corrections, $\sim A^2$, to the eigenvalues, P in Eq. (20). The neutron wave function corrections are small, $\sim A$, and are calculated by means of perturbation theory. The neutron cannot penetrate deeply inside silicon crystal, so that we have the simple expressions for the neutron wave function $\Psi(\alpha,r)$with the α of neutron spin projection along the direction of the magnetic field and near slot side $y=rD/2$

$$|\Psi(\alpha,r)\rangle=\frac{1}{\sqrt{2}}\left|\begin{matrix} exp(-ir\xi_\alpha/2)|\alpha\rangle\\ -exp(+ir\xi_\alpha/2)|\alpha\rangle\\ -\dfrac{\alpha A}{2Q}exp(+ir\xi_\alpha/2)|-\alpha\rangle\\ -\dfrac{\alpha A}{2Q}exp(-ir\xi_\alpha/2)|-\alpha\rangle \end{matrix}\right\rangle exp(iQz+iP(\alpha,r)(y-rD/2)),$$

$$\text{where } Q=\alpha\delta+\cos\xi_\alpha \text{ and } P(\alpha,r)=ir\sin\xi_\alpha \tag{21}$$

The first and second rows in (21) correspond to the incident (0) and diffracted (h) wave function components, respectively, but with the same spin projection $|\alpha\rangle$; the third and fourth rows describe the similar components but with opposite, $|-\alpha\rangle$, spin projection.

The physical meaning of Eq. (21) can be understood if we consider neutron reflection from the slot side $y=rD/2$ $(r=\pm1)$ and with the incident neutron polarization $|\beta\rangle$. The neutron wave function is

$$\Psi = \sum_{\alpha=\pm 1} d(\alpha, r)\left|\Psi(\alpha, r)\right\rangle,\quad d(\beta,r) = \sqrt{2}\exp(ir\,\xi_\beta/2),\quad d(-\beta,r) \approx \frac{\beta A}{2Q}\exp(ir(\,\xi_\beta + \xi_{-\beta})/2) \tag{22}$$

The amplitude and polarization of the reflected beam at the same slot side, y=rD/2, are expressed as

$$\Psi_h = -exp(ir\xi_\beta)\{|\beta\rangle + \frac{\beta A}{2Q}(exp(-ir\xi_\beta) + exp(ir\xi_{-\beta}))|-\beta\rangle\},\quad <\sigma_Z> = \langle\Psi_h|\sigma_Z|\Psi_h\rangle \approx \beta,$$

$$<\sigma_X> = \langle\Psi_h|\sigma_X|\Psi_h\rangle \approx \frac{\beta A}{Q}(\cos\xi_\beta + \cos\xi_{-\beta}),\quad <\sigma_Y> = \langle\Psi_h|\sigma_Y|\Psi_h\rangle \approx \frac{rA}{Q}(\sin\xi_\beta - sin\,\xi_{-\beta}) \tag{23}$$

Therefore a neutron EDM induces the small (and expected) component of neutron polarization $<\sigma_X>$ which is *parallel* to the slot axis, that is perpendicular to the crystalline electric field and the external magnetic field, **H**.
However, an EDM induces also small neutron polarization $<\sigma_Y>$ which is *parallel* to the crystalline electric field and perpendicular to **H**. What is the source of $<\sigma_Y>\neq 0$? The ordinary spin dynamic leads to the spin motion perpendicular to **H** and **E**. It is supposed in this case that the effect of spin motion is not important for neutron coordinate motion. However, in our case neutron spin transition $|\beta\rangle \rightarrow |-\beta\rangle$ changes the position of the neutron tie point inside the Darwin plateau (total reflection range), that is, the phase of the component of the wave function which is compose to the reflected beam. This last circumstance leads to the appearance of the neutron polarization component, which is parallel to the crystalline electric field and perpendicular to the slot surface. We can omit the effect of $<\sigma_Y>\neq 0$ if the absorption (emission) of the Zeeman energy leads to the small effect in the tie point position within the total reflection range, that is $|\delta|<<1$, $|\xi_\alpha - \xi_{-\alpha}|<<1$.

3.2. EDM effects in the neutron wave guidance resonator.

Theses calculations are similar to the described in point 2. However we take into account the neutron spin rotation induced by the EDM interaction in the slot walls. Let us suppose that $F_0(\alpha)$, $F_h(\alpha)$ are the components of the neutron wave function at the slot center, y=0. This wave function is written in the form at the slot side y=rD/2:

$$\Psi_S(r) = \sum_{\alpha=\pm 1}\left|\begin{matrix} F_0(\alpha)exp(iP(\alpha,0)rD/2)|\alpha\rangle \\ F_h(\alpha)exp(iP(h,0)rD/2)|\alpha\rangle \end{matrix}\right\rangle,$$

$$P(\alpha,0) = -(Q - \alpha\delta - V_0/|V_G|),\quad P(\alpha,h) = -P(\alpha,0) \tag{24a}$$

The neutron wave function should be continuous at the slot sides and $\Psi_S(r)$ can be also written as linear superposition of $|\Psi(\langle,r)\rangle$

$$\Psi_S(r) = \sum_{\alpha=\pm 1} c(\alpha,r)|\Psi(\alpha,r)\rangle =$$

$$\sum_{\alpha=\pm 1}\frac{c(\alpha,r)}{\sqrt{2}}\left|\begin{matrix} exp(-ir\xi_\alpha/2)|\alpha\rangle - \alpha A/(2Q)exp(+ir\xi_\alpha/2|-\alpha\rangle \\ -exp(ir\xi_\alpha/2)|\alpha\rangle - \alpha A/(2Q)exp(-ir\xi_\alpha/2|-\alpha\rangle \end{matrix}\right\rangle \tag{24b}$$

The numerical parameters $c(\alpha,r)$ were determined by means of comparison (24a) and (24b), so that we have 4 equations which contained only amplitudes $F_0(\alpha)$, $F_h(\alpha)$.

$$\frac{\alpha A}{2Q}(F_h(\alpha)e^{-iP(\alpha,0)rD/2+ir\xi_{-\alpha}/2} - F_0(\alpha)e^{iP(\alpha,0)rD/2-ir\xi_{-\alpha}/2}) =$$

$$F_h(-\alpha)e^{-iP(-\alpha,0)rD/2-ir\xi_{-\alpha}/2} + F_0(-\alpha)e^{iP(-\alpha,0)rD/2+ir\xi_{-\alpha}/2},\quad \alpha = \pm 1,\quad r = \pm 1 \tag{25}$$

It is convenient to introduce symmetrical and asymmetrical combination of amplitudes $F_0(\alpha)$, $F_h(\alpha)$

$$F_+(\alpha) = F_0(\alpha) + F_h(\alpha),\quad F_-(\alpha) = F_0(\alpha) - F_h(\alpha) \tag{26}$$

and to write (25) in the simple form

$$F_+(\alpha)cos(P(\alpha,0)D/2+\xi_\alpha/2)=\frac{\alpha A}{2Q}F_-(-\alpha)cos(P(-\alpha,0)D/2-\xi_\alpha/2),$$

$$F_-(\alpha)sin(P(\alpha,0)D/2+\xi_\alpha/2)=\frac{\alpha A}{2Q}F_+(-\alpha)sin(P(-\alpha,0)D/2-\xi_\alpha/2) \qquad (27)$$

Equations (27) are separated into two pairs of the equations for $F_+(1)$, $F_-(-1)$ and $F_+(-1)$, $F_-(1)$. The corresponded determinant,

$$\mathrm{detF}=\mathrm{detF_1 detF_{-1}},\ \ \mathrm{detF}=0,\ \ \mathrm{detF_\alpha}=\cos(P(\alpha,0)D/2+\xi_\alpha/2)\sin(P(-\alpha,0)D/2+\xi_{-\alpha}/2)+$$
$$A^2/(4Q^2)sin(P(\alpha,0)D/2-\xi_{-\alpha}/2)cos(P(-\alpha,0)D/2-\xi_\alpha/2) \qquad (28)$$

Without an EDM interaction with crystalline electric field, A=0, the discrete neutron modes are defined by the conditions (12), and

$$\xi_\alpha=\xi_\alpha^0,\ \ \xi_\alpha^0-D(\cos\xi_\alpha^0-V_0/|V_G|)=\pi L_\alpha,\ \ \alpha=\pm1,\ \ L_\alpha=1,2,... \qquad (29)$$

The neutron EDM induces transition between states $\alpha=1$ and $\alpha=-1$ when the momentum Q directed along slot axis is the same for state $\alpha=1$ and $\alpha=-1$,

$$cos\,\xi_\alpha-cos\,\xi_{-\alpha}=-2\alpha\delta \qquad (30)$$

The neutron EDM induces deviations of the "allowed" values ξ_α from ξ_α^0

$$\xi_\alpha=\xi_\alpha^0+\Delta\xi_\alpha,\ \ \sin\xi_\alpha^0\Delta\xi_\alpha=\sin\xi_{-\alpha}^0\Delta\xi_{-\alpha} \qquad (31)$$

These modes will be degenerate if the deviation of the Zeeman energy, $\Delta\delta$, from the value of δ^0, corresponded to this degeneracy, is small

$$\delta=\delta^0+\Delta\delta,\ \ \cos\xi_\alpha^0-\cos\xi_{-\alpha}^0=-2\alpha\delta^0 \qquad (32)$$

We find after substitution of Eqs. (29)-(32) into the equation detF=0, that

$$\Delta\xi_\alpha\,sin\,\xi_\alpha^0=r_\xi\sqrt{\frac{(1-(-1)^{L_\alpha+L_{-\alpha}})}{2}\left(\frac{A\,cos(\frac{\xi_\alpha+\xi_{-\alpha}}{2})}{QD}\right)^2+(\Delta\delta)^2}\ \ ,r_\xi=\pm1 \qquad (33)$$

We see that the neutron EDM leads to the suppression of the degeneracy of the wave guidance resonator modes which have *different* "parity" L_α and $L_{-\alpha}$. The corresponding splitting $\Delta\xi_\alpha$ ~ A/D for the case of the exact mode degeneracy, $\Delta\delta=0$. What is the source of the parameter 1/D in $\Delta\xi_\alpha$? The number of neutron reflections from slot sides is equal to the value x/D, where x is the length of neutron path along slot axis. Therefore we find that the splitting $\Delta\xi_\alpha$ ~ A/D. The neutron wave function can be found after substitution of (33) into the expressions (27)-(31).

Let us consider, for an example the case of the exact degeneracy, $\Delta\delta=0$ and $L_1=2M_1$, $L_{-1}=2M_{-1}+1$, M_1, $M_{-1}=1,2,...$ We have from the expressions (27)-(31)

$$F_0(1)=1,\ \ F_0(-1)=(-1)^{M_1+M_{-1}}r_\xi,\ \ F_h(1)=-1,\ \ F_h(-1)=(-1)^{M_1+M_{-1}}r_\xi\ ,\ \ r_\xi=\pm1 \qquad (34)$$

The amplitude of the incident component of the wave function can be written in the form

$$\Psi_0=\sum_{r_\xi}C(r_\xi)\{|+1\rangle exp(i(2\pi M_1-\xi_1^0)y/D)+|-1\rangle(-1)^{M_1+M_{-1}}r_\xi\,exp(i(2\pi M_{-1}+\pi-\xi_{-1}^0)y/D)\}\times$$

$$exp(-ir_\xi\frac{Az}{QD}cos\frac{\xi_1^0+\xi_{-1}^0}{2})exp(i(\delta^0+cos\,\xi_1^0)x) \qquad (35)$$

where $C(r_\xi)$ are the arbitrary constants (we omitted very small terms ~ $\Delta\xi_\alpha D$).

Let us suppose that the incident neutron is completely polarized along the direction of the external magnetic field at the point x=0, y=D/2. We calculated the values of $C(r_\xi)$,Ψ_0 (35) and the average value of neutron polarization at the same slot surface y=D/2 taking into account this condition. We find

$$< \sigma_z >= \cos 2\rho, \ < \sigma_x >= \sin 2\rho \cos(\frac{\xi_1^0 - \xi_{-1}^0}{2}),$$

$$< \sigma_y >= \sin 2\rho \sin(\frac{\xi_1^0 - \xi_{-1}^0}{2}), \ \rho = \frac{Ax}{QD}\cos(\frac{\xi_1^0 + \xi_{-1}^0}{2}) \tag{36}$$

We see that the direction of neutron spin can be strongly changed at the large distance, x ~QD/A, along the slot axis. The neutron spin rotates in the plane parallel to the slot surface when $\xi_1^0 \approx \xi_{-1}^0$.

4. SCHWINGER INTERACTION EFFECTS

The Neutron Spin-Orbit (Schwinger) interaction can be written in the form [2,3]

$$V_{SO}(\mathbf{G}) = -CF(\mathbf{G})\frac{\sigma[\mathbf{G} \bullet \nabla]}{bG^2}, \ C = 2\pi\mu\left(\frac{e\hbar}{mc}\right)^2 \frac{1}{v_c}(Z - f(\mathbf{G})) \tag{37}$$

where F - structural factor, b - length of scattering, μ - neutron magnetic moment, f(G) - X-ray form factor. The other symbols are standard [3]. The physical sense of the Schwinger interaction is simple: crystalline electric field **E** leads to the existence of the induced magnetic field **h**~[**E**•**v**]/c in the neutron coordinate system (**v**, c are the neutron and light speed, respectively) and the additional energy $-\mu\sigma\mathbf{h}$. The magnetic field **h** is collinear to the Z-axis in our case.

We suppose that external magnetic field is parallel to the Y-axis, that is collinear to the vector of scattering. Neutron dynamic eq-s are expressed as

$$-i\hbar^2 / m(k_0\nabla)\Psi_0 + V_0\Psi_0 + V_{-G}\Psi_h - \hbar\omega_Z\sigma_Y / 2\Psi_0 + iBV_{-G}\sigma_Z\Psi_h = 0,$$

$$-i\hbar^2 / m(k_h\nabla)\Psi_h + V_0\Psi_h + V_G\Psi_0 - \hbar\omega_Z\sigma_Y / 2\Psi_h - iBV_G\sigma_Z\Psi_0 = 0$$

$$B = \frac{CFctg\theta_B}{2bV_{-G}\sin\theta_B}, \tag{38}$$

It's well known that the following transformation doesn't change the Pauli operators relationships.

$$\sigma_X \to \sigma_Y, \ \sigma_Y \to \sigma_Z, \ \sigma_Z \to \sigma_X \tag{39}$$

The substitution (39) transforms (38) to the equations (19), but only the value of B is used instead of A Eq. (18). Therefore results for the case of Schwinger interaction will have the same form as for the case of EDM interaction if we take into account (39) and replace A→B.

5. ULTRA BACK-SCATTERING REGIME

It is supposed above that the Bragg angle isn't too close to the value of π/2, so that the ordinary two waves dynamical theory is applicable. Here we describe calculations for the case of ultra back- scattering regime when the Bragg angle $\theta_B = \pi/2$.

The neutron wave function could be written as

$$\Psi = \Psi_0 \exp(ik_0 y) + \Psi_h \exp(-ik_0 y) \tag{40}$$

$$\mathbf{k}_o = k_o(0,1,0), \ \mathbf{k}_h = k_o(0,-1,0), \ \mathbf{G} = (0_0, -2k_0, 0) \tag{41}$$

Neutron kinetic energy

$$E = \hbar^2 k_0^2 /(2m) + \Delta_l E \tag{42}$$

where $\Delta_l E$ is deviation from the exact Bragg condition. The equations of motion are written in a dimensionless form (44) after transformations (43)

$$\Psi_0 \to \Psi_0 \, exp(-ixV_0/|V_G| - i\rho_B/2), \ \ \Psi_h \to \Psi_h \, exp(-ixV_0/|V_G| + i\rho_B/2), \ \ V_G/|V_G| = exp(i\rho_B),$$

$$x \to x\frac{1}{\sqrt{k_0\Delta k_0}}, y \to y\frac{2}{\Delta k_0}, \quad \frac{\Delta k_0}{2} = \frac{m|V_G|}{\hbar^2 k_0}, \ \ \tau = 2\pi/\Delta k_0, \ \delta = \frac{\omega_Z m\tau}{\hbar\pi k_0}, \ \ \Delta_1 E = \Delta E\frac{\hbar^2 k_0 \Delta k_0}{2m} \quad (43)$$

Here the gap, Δk_0 between the dispersion surface branches doesn't contain the value of $\cos\theta_B$ (comp. with the expression (4))

$$-i\partial\Psi_0/\partial y - \partial^2\Psi_0/\partial x^2 + (-\Delta E - \delta\sigma_Z)\Psi_0 + \Psi_h + iA\sigma_Y\Psi_h = 0,$$
$$+i\partial\Psi_h/\partial y - \partial^2\Psi_h/\partial x^2 + (-\Delta E - \delta\sigma_Z)\Psi_h + \Psi_0 - iA\sigma_Y\Psi_0 = 0 \quad (44)$$

The solution of (44) is proportional to exp(iQx+iPy). It is convenient to use substitution

$$Q^2 - \alpha\delta - \Delta E = \cos\varphi_\alpha, \ \ P(\alpha, r) = ir\sin\varphi_\alpha, \ \ r = \pm 1 \quad (45)$$

The total reflection regime will exist when

$$|Q^2 - \alpha\delta - \Delta E| < 1 \quad (46)$$

Without Schwinger and EDM interactions the neutron modes are defined by the equation (47), which is similar to (12) but with the *different* value of the momentum Q directed along slot surface.

$$\varphi_\alpha = \varphi_L, \ \varphi_L - D(\cos\varphi_L - V_0/|V_G|) = \pi L, \ L = 1, 2, \ldots \quad (47)$$

Two modes with opposite spin orientation will be degenerate if

$$\cos\varphi_\alpha - \cos\varphi_{-\alpha} = -2\alpha\delta \quad (48)$$

EDM interaction removes this degeneracy and changes the value of Q at the value q

$$q = -\frac{1}{2Q}\sin\varphi_\beta\Delta\varphi_\beta = -\frac{1}{2Q}\sin\varphi_{-\beta}\Delta\varphi_{-\beta} \quad (49)$$

Splitting $\Delta\varphi_\beta$ is defined by the same expression as in Eq. (33) but with the substitution φ_α, $\varphi_{-\alpha}$ instead of ξ_α, $\xi_{-\alpha}$, respectively.

6. CONCLUSION

It was shown above the neutron wave-guidance resonator modes are discrete. It is interesting to compare Eq. (12) with the simple geometrical optics approximation for the case of thick slot, D>>1. Let us suppose that we have wave field $\Psi_0(0)$ at the slot mid. This wave will be completely reflected at the wall y=D/2, spreading up to y=-D/2, reflected once more and returns to the slot mid plane as wave

$$\Psi_0(1) = exp(-i2C_w)\Psi_0(0), \ \ C_w = D(\cos\xi - V_0/|V_G|) - \xi \quad (50)$$

We will have after N cycles

$$\Psi_0(N) = exp(-i2NC_w)\Psi_0(0) \quad (51)$$

The number of cycles, N could be very large for the case of the long slot. Therefore, the neutron wave field will be completely chaotic if conditions (12), (29) will not be fulfilled. Let us suppose that we have starting Gaussian wave packet "around" $\xi = \xi_L$ (12) and value of $\xi = \xi_L + \delta\xi$, $\delta\xi \sim 1/D$. We have the deviation of C_w

$$\delta C_w \approx -(D\sin\zeta_L + 1)\delta\zeta - 0.5D\cos\zeta_L(\delta\zeta)^2$$

This Gaussian packet will be transformed to the highly oscillatory wave function after 2N>>1 reflections; N~D if value of ξ_L isn't close to the $\pi/2$, that is to the center of the Darwin reflection plateau. The value of $N \sim D^2$ if value of $\xi_L \approx \pi/2$.

We find that the neutron EDM interaction with crystalline electric field removes discrete neutron modes degeneracy and induces beating of the neutron polarization (36) as function of coordinate along slot axis. For the case of $\xi^0_1 \approx \xi^0_{-1}$ this motion is the spin rotation in the plane parallel to the slot surface. The component of the spin motion along Y-axis is added when $\xi^0_1 \neq \xi^0_{-1}$. This unusual spin motion *along* the crystalline electric field can be understood as the result of coupling between spin and neutron coordinate dynamic in silicon. The neutron spin transition $|\beta\rangle \to |-\beta\rangle$ changes the position of neutron tie point inside the Darwin plateau, that is the phase of the component of the wave function which is corresponded to the reflected beam. This circumstance leads to the appearance of the neutron polarization component, which is parallel to the crystalline field.

Unfortunately, it is very difficult to observe these beating effects due to the extremely small value of the neutron EDM. Therefore we limit ourselves by the discussion of the regime, $\rho<<1$, that is, the initial part of these beating effects

$$<\sigma_X> \approx 2\frac{AX_1}{QD}cos(\frac{\xi_1^0+\xi_{-1}^0}{2})cos(\frac{\xi_1^0-\xi_{-1}^0}{2}) \sim 4AN,$$

$$<\sigma_Y> \approx 2\frac{AX_1}{QD}cos(\frac{\xi_1^0+\xi_{-1}^0}{2})\sin(\frac{\xi_1^0-\xi_{-1}^0}{2}), \quad N=\frac{X_1}{2D_1 ctg\theta_B} \tag{52}$$

where 2N is number on neutron reflections along the path through the slot, and X_l, D_l are the slot length and width, respectively, which are written in the dimension form. We see that the deviations, $<\sigma_X>$, $<\sigma_Y>$ of the neutron polarization is increasing along slot axis [2,3]. This accumulation of deviations exists due to the mode degeneracy in the magnetic field and was predicted by Dombeck et al. [3]. The value of A is equal to $1.6x10^{-7}$ if we suppose that $<\sigma_X>=0.01$ and N=30000. This value of A is corresponded to the value of neutron EDM, $\mu_{EDM}=4x10^{-24}$e-cm in the crystalline electric field $7.6x10^8$V/cm.
In most cases the value of slot thickness is large, D>>1 (15). Let's calculate resonance magnetic field δ^0 for the case D>>1 and near the center of Darwin plateau. By means of simple substitutions (53)

$$\frac{DV_0}{\pi|V_G|}=M+\nu, \quad L\rightarrow M+n, \quad M,n\text{-integers}, \quad n\sim 1, \quad 0<\nu<1, \quad D\cos\zeta-\zeta+\pi(n-\nu)=0, \quad \zeta\approx\pi/2 \tag{53}$$

we find decision (32,53) as an expansion over 1/D

$$cos\,\zeta \approx \frac{\pi}{2D}-\frac{U}{D}-\frac{\pi U^2}{4D^4}+\frac{2}{3}\frac{U^3}{D^4}, \quad U=\pi(n-\nu) \tag{54}$$

$$\delta^0 \approx \pi(L_\alpha - L_{-\alpha})/(2D) \tag{55}$$

Neutron time of flight from one slot side to another is approximately equal to the one half of the neutron spin Larmor procession period multiplied by the *odd* integer number (55). Only in this case the effect of neutron spin rotation by EDM interaction in slot walls is accumulated during the neutron trip along the slot axis.
The interval δQ between nearest "allowed" values of Q is equal to $\sim\pi/D$ (54). This value δQ corresponds to the distance $D_l\, ctg\theta_B$ along slot axis, that is, to the step length in the classical picture of neutron reflections from slot walls. The value of $\cos\xi$ is almost linear over n. Therefore not only pair of modes with definite parameters L_α , $L_{-\alpha}$ will be important in the neutron spin deviations, but also the other pairs of modes with the same value L_α- $L_{-\alpha}$. These additional pairs could increase $<\sigma_X>$ deviation for the case of multi mode neutron resonator, D>>1 and decreasing $<\sigma_Y>$ due to the asymmetry $<\sigma_Y>$ for the respect of transformation $\xi_1^0\leftrightarrow\xi_{-1}^0$.
As was mentioned above the calculation for the case of the Schwinger interaction is similar to the one for the case of EDM effect. The deviation of the neutron polarization is increasing along slot axis [2,3]. However parameter ρ Eq. (36) for the case of the Schwinger interaction

$$\rho=\rho_S \approx \frac{Bx_1}{D}=\frac{CF}{2bV_{-G}\sin\theta_B}\frac{x_1}{D_1} \tag{56}$$

and the small value $\cos\theta_B$ is absent in the denominator (comp. with (52)). It can be understood if we take into account that the average magnetic field **h** induced by the crystalline electric field, $<h>\sim<[E\bullet v]>\sim\cos\theta_B$ and number of reflection $\sim 1/\cos\theta_B$. The value of polarization directed along slot axis $<\sigma_X>\sim2\rho_S\sim10^{-3}X_l/D_l$ for the case of Si(440) reflection, $\theta_B\approx80^\circ$,$V_G\approx5.4*10^{-8}$eV, $C\approx10^{-10}$eV, and the external magnetic field is collinear to the Y-axis. It therefore seems that experiments can be successful.

Let us discuss some peculiarities of the neutron resonator parameters in the Ultra Back Scattering (UBS) regime. It is well known that UBS rocking curve is much wider than the ordinary rocking curve in the perfect crystal. For the case of Si (111) reflection, λ=0.627nm, $\theta_B\approx\pi$, τ=34μm and sides of the Darwin plateau are corresponded to the Q=±1 or to the angular position $\pm\sqrt{\lambda/\tau}=\pm14.8$ arc min. The energy window, corresponded to the completely reflected neutrons, $\Delta E_0\approx18.7$ MHz.
Let us consider the energy spectrum of neutrons transmitted through slot resonator in the UBS regime. The allowed neutron modes are defined by the equation (45). Their contribution in spectrum is defined by the parameters of excitation at the beginning of slot resonator. Let us suppose, for the simplicity, that all allowed modes are excited with the same probability. The normalized spectrum of the transmitted neutrons are shown at the Figure 2 for the case of slot thickness D=10, that is 108μm, and collimation Q<0.35, that is the deviation from the exact Bragg condition isn't more than 5.18 arc min. The spectrum is contained 7 peaks. The interval between nearest peaks is equal to 2.8 MHz. Probably, the selective excitation of

these modes can be achieved by means of a crystal monochromator with the FWHM of the mosaic disorientation ~1-2 arc min.

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REFERENCES

1. E.Jericha, D.E.Schwab, M.R.Jäkel,C.J.Carlile, H.Rauch, "Neutron beam tailoring by accumulation between perfect crystal mirrors", Physica B **283**, pp. 414-417, 2000.
2. K.D.Finkelstein, "Neutron spin - Pendellosüng resonance". Thesis, MIT, 1987.
3.Horne, M.A., Finkelstein, K.D., Shull, C.G., Zeilinger, A. & Bernstein, H.J., "Neutron spin - Pendellšsung resonance", Physica B **151**, 189-192, 1988.
4. T. Dombeck, H.Kaiser, D. Koetke, M. Peshkin and R. Ringo , "A Bragg Scattering Method to Search for the Neutron Electric Dipole Moment", Phy-9814-TH-2001, Argonne National Laboratory, March 2001.
5. Z.G. Pinsker, "Dynamical Scattering of X-Rays in Crystals", Springer-Verlag, Berlin, 1978.
6. H.Rauch and S.Werner, "Neutron Interferometry", Oxford University Press, 2000.
7. C.G.Shull, "Neutron spin-neutron orbit interaction with slow neutrons", Phys. Rev. Let. **10**,297-298,1963.

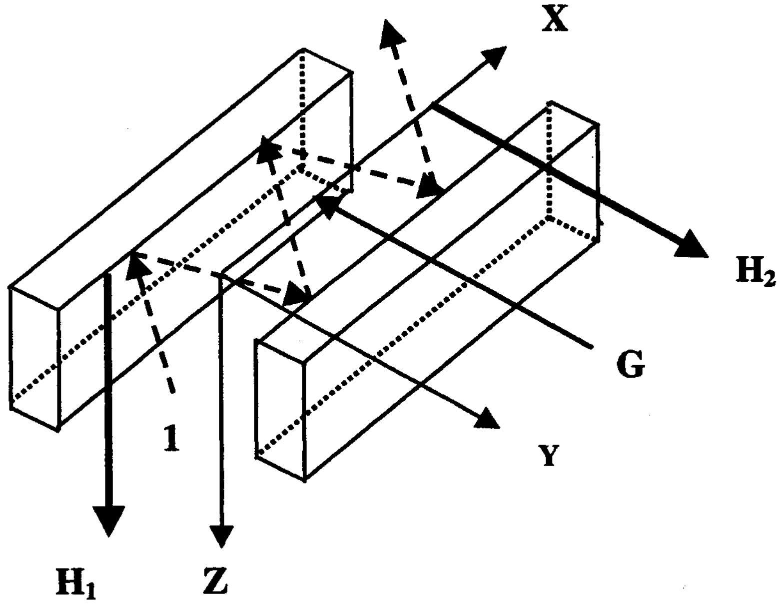

Figure 1. Neutron Wave Guidance – Resonator. 1- neutron trajectory inside slot cut in the perfect Si single crystal. G – scattering vector. H_1, H_2 – the external magnetic field for the case of EDM and Schwinger interaction studies, respectively.

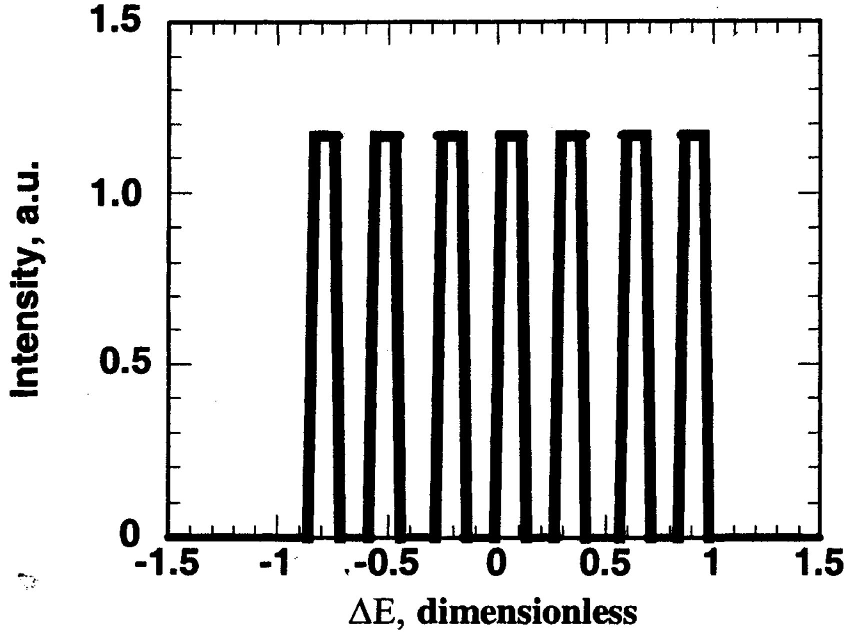

Figure 2. Energy spectrum of neutrons transmitted through slot resonator. Ultra back scattering regime. Si(111). Slot thickness D=10, beam collimation $Q \leq 0.35$ The value of $\Delta E=1$ is corresponded to the frequency 9.35 MHz. The energy "window" is spreading from $\Delta E = -1$ to $\Delta E=1$ for the case of the "ordinary" UBS crystal analyzer.